INFLUENCE OF SPIN-ORBIT QUENCHING ON THE SOLVATION OF INDIUM IN HELIUM DROPLETS

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Recent experimental interest of the collaborating group of M. Koch on the dynamics of electronic excitations of indium in helium droplets triggered a series of computational studies on the group 13 elements Al, Ga and In and their indecisive behavior between wetting and non wetting when placed onto superfluid helium droplets. We employ a combination of multiconfigurational self consistent field calculations (MCSCF) and multireference configuration interaction (MRCI) to calculate the diatomic potentials. Particularly interesting is the case of indium with an Ancilotto parameter[a] λ close to the threshold value of 1.9.

As shown by Reho et al.[b] the spin-orbit splitting of metal atoms solvated in helium droplets is subject to a quenching effect. This can drastically change the solvation behavior. In this work we extend the approach presented by Reho et al. to include distance dependent spin-orbit coupling. The resulting potential surfaces are used to calculate the solvation energy of the ground state and the first excited state with orbital-free helium density functional theory.

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[a] F. Ancilotto, P. B. Lerner and M. W. Cole, *Journal of Low Temperature Physics*, 1995, **101**, 1123-1146

[b] J. H. Reho, U. Merker, M. R. Radcliff, K. K. Lehmann and G. Scoles, *The Journal of Physical Chemistry A*, 2000, **104**, 3620-3626